N,N-Dimethylformamide 68-12-2 | DTXSID6020515

Model Performance

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Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 9.24 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.45e-01

Confidence level: 5.90e-01

Nearest Neighbors from the Training Set

Image not found

Diethylacetamide Measured: 69.2 Predicted: 64.5 Image not found

Acrylamide Measured: 50.1 Predicted: 16.7 Image not found

1,2-Propylene glycol Measured: 2.29 Predicted: 4.24

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Acetamide Measured: 5.01 Predicted: 4.44 Image not found

Acetic acid
Measured: 1.00
Predicted: 2.40